



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 05:20 PM EST

PDB ID : 2EAC
Title : Crystal structure of 1,2- α -L-fucosidase from *Bifidobacterium bifidum* in complex with deoxyfuconojirimycin
Authors : Nagae, M.; Tsuchiya, A.; Katayama, T.; Yamamoto, K.; Wakatsuki, S.; Kato, R.
Deposited on : 2007-01-31
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

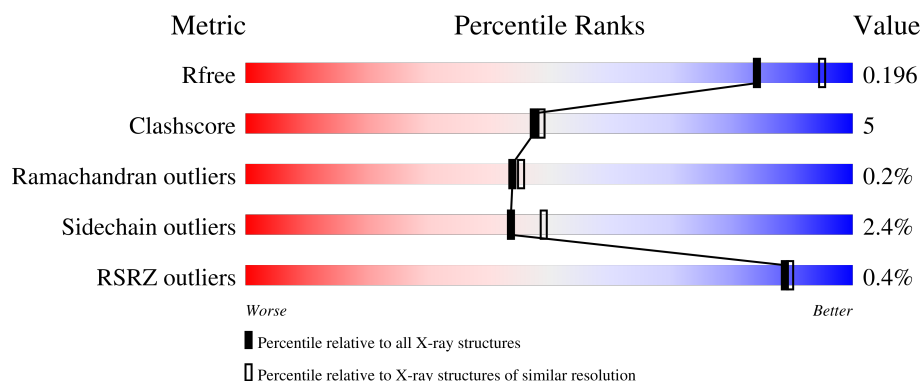
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	899	 88% 8% ..
1	B	899	 87% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15171 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	881	Total	C	N	O	S	0	0	0
			6719	4183	1161	1360	15			
1	B	885	Total	C	N	O	S	0	0	0
			6743	4196	1165	1367	15			

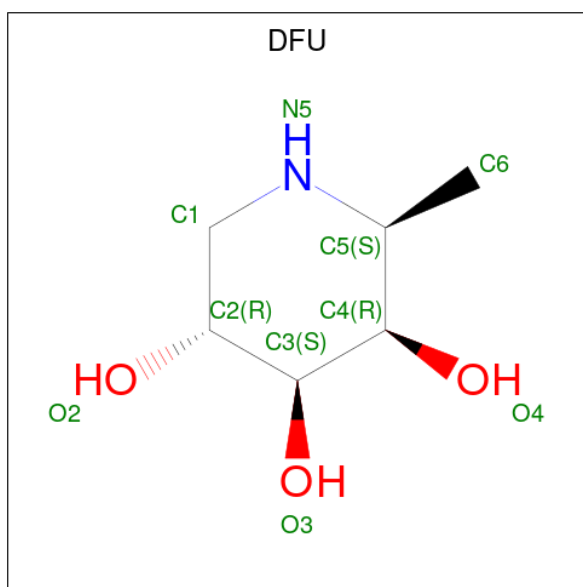
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q6JV24
B	0	MET	-	initiating methionine	UNP Q6JV24

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is (2S,3R,4S,5R)-2-METHYLPYPERIDINE-3,4,5-TRIOL (three-letter code: DFU) (formula: C₆H₁₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		
3	B	1	Total	C	N	O	0	0
			10	6	1	3		

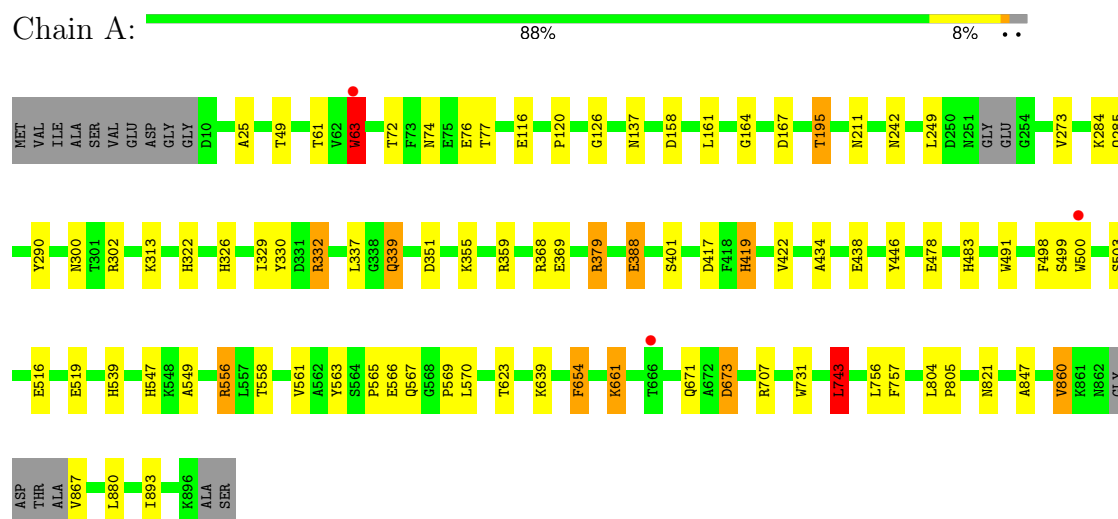
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	896	Total	O	0	0
			896	896		
4	B	789	Total	O	0	0
			789	789		

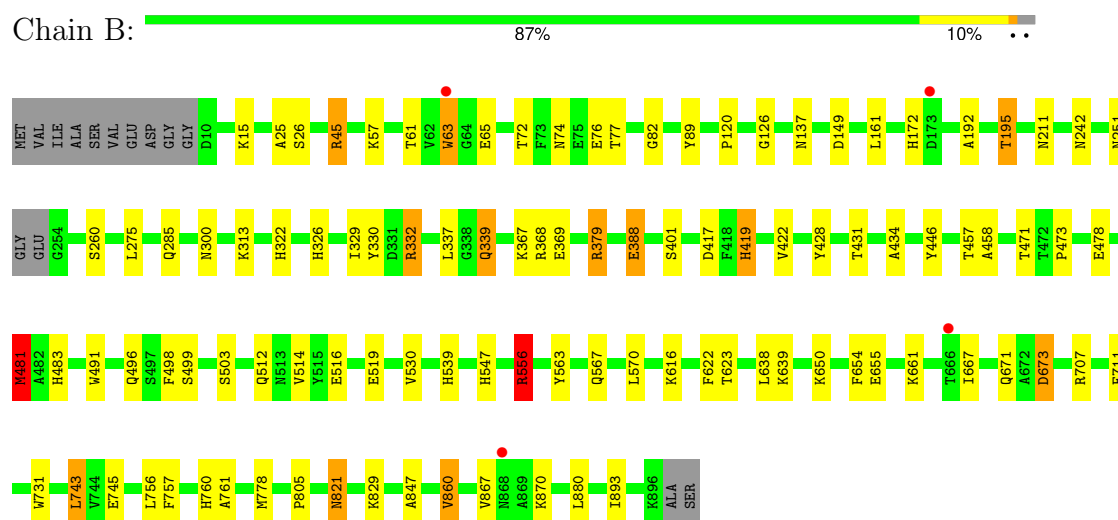
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alpha-fucosidase



• Molecule 1: Alpha-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.67Å 111.70Å 98.35Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	48.97 – 2.10 48.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.97-2.10) 100.0 (48.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.150 , 0.198 0.151 , 0.196	Depositor DCC
R_{free} test set	5692 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15171	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DFU, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	3/6863 (0.0%)	0.80	10/9332 (0.1%)
1	B	0.75	1/6888 (0.0%)	0.78	11/9368 (0.1%)
All	All	0.76	4/13751 (0.0%)	0.79	21/18700 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	GLU	CG-CD	5.60	1.60	1.51
1	A	388	GLU	CD-OE2	5.44	1.31	1.25
1	A	388	GLU	CG-CD	5.07	1.59	1.51
1	A	63	TRP	CE3-CZ3	-5.04	1.29	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ARG	NE-CZ-NH2	-18.39	111.11	120.30
1	B	379	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	A	379	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	B	332	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	B	332	ARG	NE-CZ-NH2	-11.69	114.46	120.30
1	B	379	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	A	332	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	332	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	A	379	ARG	CD-NE-CZ	6.70	132.98	123.60
1	B	556	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	A	673	ASP	C-N-CA	-6.51	105.42	121.70
1	A	351	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	743	LEU	CA-CB-CG	-6.13	101.20	115.30
1	A	556	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	A	368	ARG	NE-CZ-NH2	-5.76	117.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	368	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	673	ASP	C-N-CA	-5.50	107.94	121.70
1	B	481	MET	CG-SD-CE	5.39	108.83	100.20
1	B	379	ARG	CD-NE-CZ	5.38	131.14	123.60
1	B	556	ARG	NE-CZ-NH2	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6719	0	6400	65	0
1	B	6743	0	6420	79	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	13	0	0
3	B	10	0	13	0	0
4	A	896	0	0	8	0
4	B	789	0	0	14	0
All	All	15171	0	12846	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:HD22	1:B:211:ASN:HD22	1.06	0.94
1:A:63:TRP:HZ3	1:A:72:THR:HG1	0.94	0.91
1:A:313:LYS:HD2	4:A:2556:HOH:O	1.70	0.91
1:B:63:TRP:HZ3	1:B:72:THR:OG1	1.53	0.91
1:A:137:ASN:HD22	1:A:211:ASN:HD22	1.22	0.86
1:A:242:ASN:HD21	1:A:300:ASN:HD22	1.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ARG:HH12	1:B:639:LYS:HB2	1.45	0.82
1:B:63:TRP:HZ3	1:B:72:THR:HG1	0.82	0.80
1:A:63:TRP:HZ3	1:A:72:THR:OG1	1.65	0.80
1:B:458:ALA:HA	1:B:481:MET:HE2	1.64	0.79
1:B:137:ASN:ND2	1:B:211:ASN:HD22	1.80	0.79
1:B:379:ARG:CD	1:B:434:ALA:HB1	2.13	0.79
1:B:337:LEU:H	1:B:339:GLN:HE22	1.30	0.77
1:A:417:ASP:OD1	1:A:419:HIS:HD2	1.69	0.76
1:A:337:LEU:H	1:A:339:GLN:HE22	1.34	0.76
1:A:556:ARG:NH1	1:A:639:LYS:O	2.19	0.73
1:A:161:LEU:O	1:A:326:HIS:HE1	1.72	0.73
1:A:483:HIS:HD2	1:A:503:SER:H	1.33	0.73
1:A:330:TYR:O	1:A:379:ARG:NH2	2.22	0.72
1:A:339:GLN:HE21	1:A:339:GLN:H	1.36	0.72
1:B:483:HIS:HD2	1:B:503:SER:H	1.37	0.71
1:B:137:ASN:HD22	1:B:211:ASN:ND2	1.85	0.71
1:B:458:ALA:HA	1:B:481:MET:CE	2.21	0.71
1:B:539:HIS:HD2	4:B:2176:HOH:O	1.74	0.70
1:B:242:ASN:HD21	1:B:300:ASN:HD22	1.39	0.70
1:A:379:ARG:HD2	1:A:434:ALA:HB1	1.73	0.69
1:B:74:ASN:HD21	1:B:401:SER:H	1.41	0.69
1:A:379:ARG:CD	1:A:434:ALA:HB1	2.22	0.68
1:B:313:LYS:HD2	4:B:2476:HOH:O	1.95	0.65
1:A:567:GLN:NE2	1:A:671:GLN:H	1.94	0.65
1:B:379:ARG:HD2	1:B:434:ALA:HB1	1.78	0.65
1:B:379:ARG:HD3	1:B:434:ALA:HB1	1.78	0.64
1:B:860:VAL:HG22	1:B:867:VAL:HB	1.80	0.64
1:A:539:HIS:HD2	4:A:2293:HOH:O	1.80	0.63
1:B:707:ARG:NH2	4:B:1899:HOH:O	2.32	0.63
1:B:567:GLN:NE2	1:B:671:GLN:H	1.98	0.62
1:B:161:LEU:O	1:B:326:HIS:HE1	1.83	0.62
1:A:195:THR:CG2	4:A:1703:HOH:O	2.49	0.61
1:B:556:ARG:NH1	1:B:639:LYS:HB2	2.13	0.60
1:A:285:GLN:HE22	1:A:446:TYR:HA	1.66	0.60
1:B:731:TRP:CD1	1:B:743:LEU:HD13	2.36	0.60
1:B:417:ASP:OD1	1:B:419:HIS:HD2	1.84	0.60
1:A:137:ASN:ND2	1:A:211:ASN:HD22	1.96	0.60
1:B:25:ALA:HB3	1:B:63:TRP:CD1	2.36	0.60
1:B:26:SER:HA	1:B:45:ARG:HD2	1.84	0.60
1:A:249:LEU:HD23	1:A:273:VAL:HG12	1.83	0.59
1:A:302:ARG:NH1	4:A:2241:HOH:O	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLN:HE22	1:B:446:TYR:HA	1.66	0.59
1:A:339:GLN:H	1:A:339:GLN:NE2	2.01	0.59
1:A:25:ALA:HB3	1:A:63:TRP:CD1	2.40	0.57
1:A:74:ASN:HD21	1:A:401:SER:H	1.51	0.57
1:A:120:PRO:HB2	1:A:498:PHE:CD1	2.40	0.57
1:B:337:LEU:H	1:B:339:GLN:NE2	1.99	0.56
1:A:499:SER:HB3	1:A:570:LEU:HD21	1.88	0.56
1:B:63:TRP:CZ3	1:B:72:THR:OG1	2.41	0.56
1:B:499:SER:HB3	1:B:570:LEU:HD21	1.88	0.56
1:A:332:ARG:HD3	4:A:2323:HOH:O	2.06	0.55
1:A:707:ARG:NH1	4:A:2379:HOH:O	2.38	0.55
1:A:483:HIS:CD2	1:A:503:SER:H	2.20	0.55
1:B:483:HIS:CD2	1:B:503:SER:H	2.22	0.55
1:B:457:THR:O	1:B:481:MET:HE3	2.07	0.55
1:A:355:LYS:NZ	1:A:359:ARG:NE	2.55	0.54
1:A:671:GLN:O	1:A:673:ASP:O	2.26	0.54
1:B:251:ASN:HB2	4:B:2227:HOH:O	2.07	0.54
1:B:671:GLN:O	1:B:673:ASP:O	2.26	0.54
1:A:161:LEU:O	1:A:326:HIS:CE1	2.59	0.53
1:A:867:VAL:HA	4:A:2119:HOH:O	2.08	0.53
1:A:355:LYS:HZ3	1:A:359:ARG:HE	1.57	0.53
1:B:870:LYS:HE3	4:B:1827:HOH:O	2.08	0.53
1:B:650:LYS:HE2	1:B:655:GLU:O	2.09	0.52
1:B:330:TYR:O	1:B:379:ARG:NH2	2.41	0.52
1:A:25:ALA:HB1	1:A:49:THR:OG1	2.10	0.52
1:A:731:TRP:CD1	1:A:743:LEU:HD13	2.44	0.51
1:B:322:HIS:HD2	4:B:1829:HOH:O	1.92	0.51
1:B:847:ALA:HB1	1:B:880:LEU:HD13	1.91	0.51
1:B:339:GLN:HE21	1:B:339:GLN:H	1.58	0.51
1:A:76:GLU:HG3	1:A:77:THR:HG23	1.93	0.51
1:A:116:GLU:OE1	1:A:661:LYS:HE3	2.12	0.50
1:B:76:GLU:HG3	1:B:77:THR:HG23	1.94	0.50
1:A:847:ALA:HB1	1:A:880:LEU:HD13	1.94	0.50
1:A:860:VAL:HB	1:A:893:ILE:HG12	1.92	0.49
1:A:355:LYS:NZ	1:A:359:ARG:HE	2.09	0.49
1:B:498:PHE:HE2	1:B:563:TYR:HB2	1.78	0.49
1:A:337:LEU:H	1:A:339:GLN:NE2	2.08	0.49
1:A:417:ASP:OD1	1:A:419:HIS:CD2	2.58	0.49
1:A:478:GLU:OE1	1:A:539:HIS:HE1	1.96	0.49
1:B:329:ILE:O	1:B:332:ARG:HG3	2.13	0.49
1:B:556:ARG:NH1	1:B:639:LYS:O	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:GLU:HA	1:B:519:GLU:HB2	1.95	0.48
1:B:367:LYS:NZ	1:B:745:GLU:OE1	2.34	0.47
1:B:120:PRO:HB2	1:B:498:PHE:CE1	2.50	0.47
1:A:126:GLY:HA2	1:A:491:TRP:CZ2	2.50	0.47
1:B:326:HIS:HD2	4:B:1808:HOH:O	1.96	0.47
1:A:329:ILE:O	1:A:332:ARG:HG3	2.14	0.47
1:B:57:LYS:HD2	4:B:2085:HOH:O	2.14	0.47
1:B:499:SER:O	1:B:563:TYR:CE2	2.68	0.47
1:B:829:LYS:HD3	1:B:829:LYS:HA	1.74	0.47
1:A:516:GLU:HA	1:A:519:GLU:HB2	1.96	0.47
1:A:74:ASN:ND2	1:A:401:SER:H	2.12	0.46
1:A:355:LYS:HG2	1:A:359:ARG:HE	1.81	0.46
1:B:778:MET:CE	1:B:805:PRO:HG3	2.46	0.46
1:A:120:PRO:HB2	1:A:498:PHE:CE1	2.49	0.46
1:B:661:LYS:NZ	4:B:2219:HOH:O	2.48	0.46
1:B:149:ASP:O	1:B:172:HIS:HE1	1.99	0.46
1:B:74:ASN:ND2	1:B:401:SER:H	2.11	0.46
1:A:438:GLU:HG3	4:A:1984:HOH:O	2.16	0.46
1:B:326:HIS:CD2	4:B:1808:HOH:O	2.68	0.46
1:A:164:GLY:O	1:A:322:HIS:HE1	1.98	0.45
1:A:498:PHE:HE2	1:A:563:TYR:HB2	1.81	0.45
1:B:471:THR:O	1:B:473:PRO:HD3	2.16	0.45
1:B:195:THR:CG2	4:B:1985:HOH:O	2.65	0.45
1:A:498:PHE:CE2	1:A:563:TYR:HB2	2.52	0.45
1:B:499:SER:O	1:B:563:TYR:CD2	2.70	0.45
1:A:549:ALA:HB2	1:A:558:THR:HG23	1.99	0.45
1:A:860:VAL:HG22	1:A:867:VAL:HB	1.98	0.45
1:B:126:GLY:HA2	1:B:491:TRP:CZ2	2.52	0.45
1:A:565:PRO:HA	1:A:566:GLU:HA	1.79	0.45
1:A:63:TRP:CZ3	1:A:72:THR:OG1	2.52	0.45
1:B:15:LYS:HB2	4:B:2169:HOH:O	2.16	0.44
1:A:339:GLN:HB2	1:A:369:GLU:HA	1.99	0.44
1:B:496:GLN:NE2	4:B:2271:HOH:O	2.51	0.43
1:A:567:GLN:HE21	1:A:671:GLN:H	1.61	0.43
1:B:192:ALA:HB3	1:B:275:LEU:HB2	2.01	0.42
1:B:707:ARG:O	1:B:711:PHE:HB2	2.19	0.42
1:B:760:HIS:N	1:B:761:ALA:HA	2.34	0.42
1:B:512:GLN:O	1:B:516:GLU:HG3	2.19	0.42
1:A:284:LYS:O	1:A:290:TYR:HA	2.19	0.41
1:B:339:GLN:HB2	1:B:369:GLU:HA	2.01	0.41
1:B:82:GLY:HA2	1:B:89:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LYS:HG3	1:B:667:ILE:HG12	2.02	0.41
1:B:860:VAL:HB	1:B:893:ILE:HG12	2.03	0.41
1:B:63:TRP:HB3	1:B:65:GLU:HG2	2.03	0.41
1:B:428:TYR:HA	1:B:431:THR:OG1	2.21	0.41
1:B:285:GLN:NE2	4:B:1726:HOH:O	2.52	0.41
1:B:478:GLU:OE1	1:B:539:HIS:HE1	2.03	0.41
1:B:498:PHE:CE2	1:B:563:TYR:HB2	2.56	0.41
1:A:569:PRO:HG2	1:A:654:PHE:HZ	1.86	0.41
1:B:339:GLN:NE2	1:B:339:GLN:H	2.18	0.41
1:B:556:ARG:NH1	1:B:638:LEU:O	2.54	0.41
1:A:158:ASP:OD1	1:A:167:ASP:OD2	2.39	0.41
1:B:514:VAL:HG12	1:B:530:VAL:HG12	2.03	0.40
1:A:355:LYS:HZ1	1:A:359:ARG:NE	2.19	0.40
1:A:804:LEU:HD12	1:A:805:PRO:HD2	2.03	0.40
1:B:616:LYS:HE3	1:B:622:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	875/899 (97%)	846 (97%)	27 (3%)	2 (0%)	44	45
1	B	881/899 (98%)	856 (97%)	23 (3%)	2 (0%)	44	45
All	All	1756/1798 (98%)	1702 (97%)	50 (3%)	4 (0%)	44	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	VAL
1	A	500	TRP
1	B	422	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	821	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	701/712 (98%)	685 (98%)	16 (2%)	45	51
1	B	703/712 (99%)	685 (97%)	18 (3%)	41	46
All	All	1404/1424 (99%)	1370 (98%)	34 (2%)	44	49

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	63	TRP
1	A	195	THR
1	A	339	GLN
1	A	388	GLU
1	A	419	HIS
1	A	547	HIS
1	A	561	VAL
1	A	623	THR
1	A	654	PHE
1	A	661	LYS
1	A	743	LEU
1	A	756	LEU
1	A	757	PHE
1	A	821	ASN
1	A	860	VAL
1	B	45	ARG
1	B	61	THR
1	B	63	TRP
1	B	195	THR
1	B	260	SER
1	B	339	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	388	GLU
1	B	419	HIS
1	B	481	MET
1	B	547	HIS
1	B	556	ARG
1	B	623	THR
1	B	654	PHE
1	B	743	LEU
1	B	756	LEU
1	B	757	PHE
1	B	821	ASN
1	B	860	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	93	ASN
1	A	100	ASN
1	A	134	ASN
1	A	137	ASN
1	A	213	ASN
1	A	285	GLN
1	A	300	ASN
1	A	322	HIS
1	A	326	HIS
1	A	339	GLN
1	A	342	HIS
1	A	397	GLN
1	A	419	HIS
1	A	483	HIS
1	A	513	ASN
1	A	539	HIS
1	A	543	ASN
1	A	567	GLN
1	A	587	ASN
1	A	821	ASN
1	A	841	ASN
1	B	74	ASN
1	B	93	ASN
1	B	100	ASN
1	B	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	137	ASN
1	B	172	HIS
1	B	213	ASN
1	B	251	ASN
1	B	285	GLN
1	B	300	ASN
1	B	322	HIS
1	B	326	HIS
1	B	339	GLN
1	B	342	HIS
1	B	397	GLN
1	B	419	HIS
1	B	483	HIS
1	B	513	ASN
1	B	539	HIS
1	B	543	ASN
1	B	567	GLN
1	B	587	ASN
1	B	695	ASN
1	B	821	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DFU	B	1691	-	10,10,10	0.94	1 (10%)	12,14,14	1.14	1 (8%)
3	DFU	A	1690	-	10,10,10	0.63	0	12,14,14	1.17	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DFU	B	1691	-	-	-	0/1/1/1
3	DFU	A	1690	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1691	DFU	C1-C2	2.02	1.54	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1690	DFU	C1-N5-C5	3.60	118.62	109.48
3	B	1691	DFU	C1-N5-C5	3.18	117.56	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	881/899 (97%)	-0.83	3 (0%) 90 91	6, 13, 27, 41	0
1	B	885/899 (98%)	-0.67	4 (0%) 87 88	7, 16, 32, 47	0
All	All	1766/1798 (98%)	-0.75	7 (0%) 89 90	6, 14, 30, 47	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	666	THR	3.1
1	B	868	ASN	2.9
1	B	666	THR	2.4
1	A	500	TRP	2.4
1	A	63	TRP	2.3
1	B	63	TRP	2.1
1	B	173	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DFU	A	1690	10/10	0.96	0.06	11,16,19,20	0
3	DFU	B	1691	10/10	0.96	0.06	12,16,18,22	0
2	CA	A	899	1/1	0.98	0.13	22,22,22,22	0
2	CA	A	900	1/1	0.99	0.04	20,20,20,20	0
2	CA	B	900	1/1	0.99	0.10	20,20,20,20	0
2	CA	B	899	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.